CHAPTER II
BACKGROUND AND LITERATURE SURVEY

2.1 Background

2.1.1 Basic Elements of Multi-objective Optimization

The basic theory of basic multi-objective optimization is briefly discussed by classifying into each below category (Rodera, Bagajewicz and Trafails, 2002).

2.1.1.1 Formulation of Multi-objective Optimization

When there are q objectives to be optimized simultaneously with n constrained function, the mathematical problem can be formulated as follows

$$\max z_l = f_l(x) \qquad l = 1,2,\ldots,q \tag{2.1}$$

subject to

$$g_i(x) \leq a_i \qquad i = 1,2,\ldots,n \tag{2.2}$$

where z is the objective value, f(x) is the objective function, and g(x) is the constrained function and x is a vector of n nonnegative real numbers.

2.1.1.2 Optimal and Efficient Points

In the classical sense, a maximum (optimal) solution is the one that attains the maximum value of all of the objectives concurrently. The point x^* is optimal for the problem defined if and only if $x^* \in S$ and $f_l(x^*) \geq f_l(x)$ for all l and for all $x \in S$, where S is the feasible region. Thus, generally, there is no optimal solution to a multi-objective optimization problem. Therefore, it can be satisfied with obtaining only the efficient solutions.

An efficient solution, also called a noninferior or Pareto optimal solution, is one in which no increase can be attained in any of the objectives without causing a simultaneous decrease in at least one of the objectives. The solution x^* is efficient for the problem defined if and only if there exists no x in S such that $f_l(x) \geq f_l(x^*)$ for all l and $f_l(x) \geq f_l(x^*)$ for at least one l.

2.1.1.3 Aspiration Levels

Objective function values, which are satisfactory or desirable to the decision maker, are called aspiration levels and they are denoted by $\bar{z}_i$, i = 1, ..., p. The vector $\bar{z}_i \in R^p$ consisting of aspiration levels is called a reference point.

2.1.1.4 Ranges of the Pareto Set

For this step, the ranges of the set of Pareto optimal solutions are investigated. It assumes that the objective functions are bounded over the feasible region S. An objective vector maximizing each of the objective functions is called an ideal (or perfect) objective vector z*. The components of the ideal objective vector z* are obtained by solving the following p problems

$$\max f_l(x) \quad (2.3)$$

subject to

$$x \in S \text{ for } l = 1,\ldots,p \quad (2.4)$$

Usually, the ideal objective vector is not feasible because there are some conflicts among the objectives. Even though, it can be considered a reference point. In practice, especially, in the case of nonconvex problems, the definition of the ideal vector assumes that we know the global minima of the individual objective functions, which is not that simple.

The lower bound vector of the Pareto optimal set is the so-called nadir objective vector, which can be estimated from a payoff table.

2.1.1.5 Point-estimate Weighed-sums Approach

Next, we define the P_λ problem and describe the so-called point-estimate weighed-sums approach. By using this approach, it must transform the original multi-objective optimization problem into a single-objective parametric optimization problem. The method is as follows: each objective is multiplied by a strictly positive scalar λ_i. Then, the p weighed objectives are summed to form a weighed-sums objective function. Without loss of generality, it assumes that each weighing vector $\lambda \in R^p$ is normalized so that its components sum to 1. By solving the following P_λ problem, one hopes that an optimal solution will be produced. Thus, the P problem is

$$(MOP)\ \{\max\ (f_1(x),\ldots, f_p(x)),\ \text{s.t. } x \in S\}$$

$$\Leftrightarrow$$

$$(P_\lambda)\ \{\max\ (\lambda_1 f_1(x)+ \lambda_2 f_2(x)+\ldots+ \lambda_p f_p(x)),\ \text{s.t. } x \in S,\ {}^{p}\textstyle\sum_{i=1}\lambda_i = 1,\ \lambda_1 > 0\} \quad (2.5)$$

2.1.1.6 Tchebycheff Method

This topic is another approach that can be used effectively in the optimization problem effectively. The Tchebycheff method has been designed to be user-friendly for the decision maker. Specifically, the distance from the ideal objective vector measured by a weighed Tchebycheff metric is minimized. Different solutions are obtained with different weighing vectors in the metric. The solution space is reduced by working with sequences of smaller and smaller subsets of the weighting vector spaces. The idea is to develop a sequence of progressively smaller subsets of the Pareto optimal set until the best compromise solution is found. At each different iteration, different objective vectors are presented to the decision maker, and he is asked to select the most preferred solution. The feasible region is reduced, and new alternatives from the reduced space are presented to the decision maker for selection. However, there is a difference in the way weighting vectors are employed. Instead of using weighting vectors $\lambda = \{\lambda \in R^p: \lambda_i > 0, {}^{p}\sum_{i=1}\lambda_i = 1\}$ as in the point-estimate weighed-sums approach, weighing vectors $\lambda = \{\lambda \in R^p: \lambda_i \geq 0, {}^{p}\sum_{i=1}\lambda_i = 1\}$ are used to define different Tchebycheff metrics. Therefore, the Tchebycheff method has the following advantages. (a) It can converge to nonextreme optimal solutions in linear multiobjective optimization. (b) The method can compute unsupported and improperly nondominated criterion vectors. This makes the method generalizable to integer and nonlinear multi-objective optimization. (c) The method uses conventional single-objective mathematical programming software.

2.1.1.7 Two-Stage Decision Making Stochastic Models

The two-stage stochastic programming problems (Dantzig, 1955; Beale, 1955) are characterized by two essential features: the uncertainty in the problem data and the sequence of decisions. Some of the model parameters are considered random variables with a certain probability distribution. In turn, some decisions are taken at the planning stage, that is, before the uncertainty is revealed, while a number of other decisions can only be made after the uncertain data becomes known. The first class of decisions is called the first-stage decisions. On the other hand, the decisions made after the uncertainty is unveiled are called second-stage or recourse decisions. First stage decisions are structural and often consist of capital investment, while second-stage decisions are often operational. Planning process capacity expansions under uncertainty are one type of systems widely studied using these techniques (Murphy et al., 1982; Eppen et al., 1989; Sahinidis et al., 1989; Berman and Ganz, 1994; Lui and Sahinidis, 1996; Ahmed and Sahinidis, 2000).

Any decision to buy and allocate resources or build a plant "here and now", that is, at the planning time, is a first stage decision. Any other decision that is taken at a later time is a second stage decision. Yet, some structural decisions corresponding to a future time can be considered as a second-stage, that is, one may want to wait until some uncertainty (not necessarily all) is realized to make additional structural decisions (handled through the so-called multi-stage models). The general extensive form of a two-stage mixed-integer linear stochastic problem with fixed recourse and a finite number of scenarios is (Birge and Louveaux, 1997):

$$\text{Model SP: } \max E[\text{profit}] = p_s q^t_s y_s \quad (2.6)$$

subject to

$$Ax = b \quad (2.7)$$

$$c^t_1 x + c^t_2 y_s < C \quad (2.8)$$

$$T_s x + W y_s = h_s \quad \forall s \in S \quad (2.9)$$

where x represents the first-stage mixed-integer decision variables and y_s are the second-stage variables corresponding to scenario s, which has probability p_s. The uncertain parameters in this model appear in the coefficients q_s, the matrix T_s, the recourse matrix W, and in the independent terms h_s.

However, model SP does not provide any control over the variability of the profit over the different scenarios. For example, consider the histogram of two feasible solutions of a project shown in Figure 2.1. The first case has a larger expected profit (3.38) than the second one (3.35); however, one can argue that Case I is riskier than Case II. Indeed, if one defines risk as the probability of profit to be smaller than a certain number, then one can conclude that Case I contains several scenarios where a small profit is expected. Therefore, a risk-averse decision maker would prefer Case II. Nevertheless, all this depends on the profit expectation level chosen. For example, if risk is now thought of as the probability of having a profit of 7 or more, then Case II is riskier. However, a risk-averse decision maker will always prefer to look at the lower value of profit target than at a larger one.

This kind of preferences cannot be taken into account by using the straight stochastic model. Then, a proper measure of financial risk needs to be included.

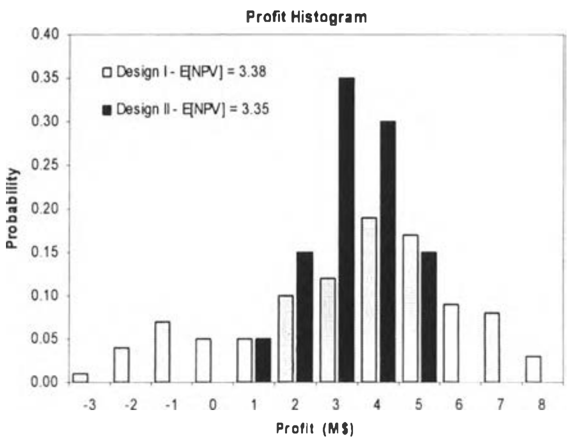

Figure 2.1 Profit histogram for two cases of resource allocation.

2.1.2 <u>Financial Risk</u>

The financial risk associated with a planning project under uncertainty risk is defined as the probability of not meeting a certain target objective function level referred to as Ω. That is, the risk constituted with a design x and a target Ω is therefore expressed by the following probability (Figure2.2):

$$\text{Risk}(x,\Omega) = P(\text{Profit}(x) < \Omega) \quad (2.10)$$

where Profit(x) is the actual profit, i.e., the profit result after the uncertainty has been unvieled and a scenario realized.

Since profit can be related to a summation over a set of independent scenarios, we have

$$\text{Risk}(x,\Omega) = \sum_{s\in S} p_s z_s(x,\Omega) \quad (2.11)$$

where $z_s(x,\Omega)$ is a new binary variable that takes the value of 1, when $\text{Profit}_s(x) < \Omega$, and zero otherwise.

This equation constitutes a formal definition of financial risk for two-stage stochastic problems. When profit has a continuous probability distribution, financial risk –defined as the probability of not meeting a target profit (Ω), can be express as:

$$\text{Risk}(x,\Omega) = \int_{-\infty}^{\Omega} f(x,\xi)d\xi \quad (2.12)$$

where $f(x,\xi)$ is the profit probability distribution function.

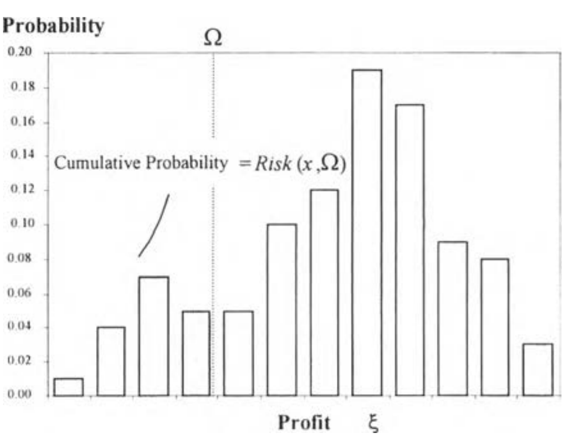

Figure 2.2 Definition of risk (Discrete Case).

A more straightforward way of assessing and understanding the trade-offs between risk and profit is to use the cumulative risk curve, as depicted in Figure 2.3 for the continuous case, which is the limit for a large number of scenarios.

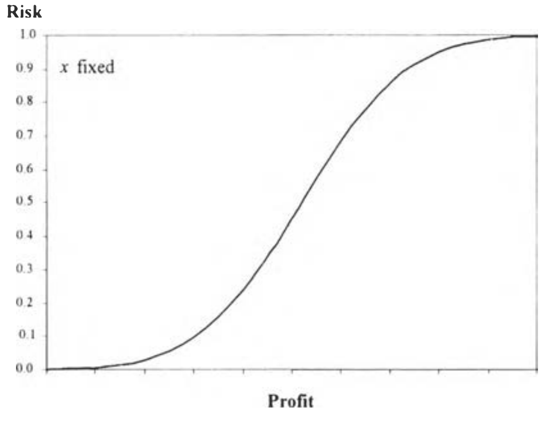

Figure 2.3 Risk curve (Continuous case).

In order to illustrate the usefulness of the above multi-objective formulation, consider a set of hypothetical solutions as depicted in Figure 2.4. Solutions 2 and 3 maximize the expected profit with minimum financial risk at targets Ω_2 and Ω_1, respectively. Thus, minimizing risk at each target independently of others targets results in designs that perform well around the specific target but do poorly in the rest of the range. When risk, on the other hand, is minimized for every target at the same time, solutions that perform well in the entire range of interest may be found. Barbaro and Bagajewicz (2003) proposed a multiobjective methodology to generate all these curves. This methodology uses either a multiparametric approach, or a penalty function approach. Both guarantee pareto-optimality.

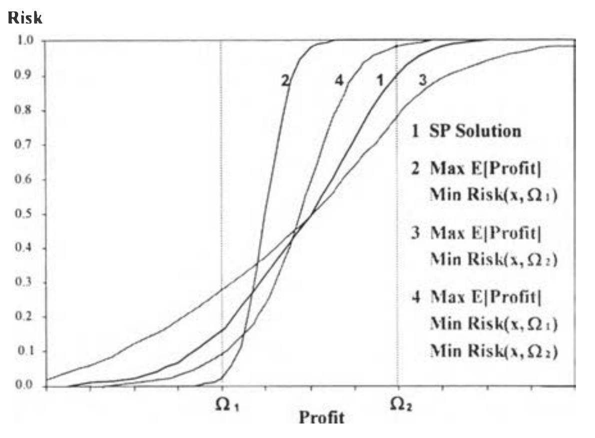

Figure 2.4 Spectrum of solutions.

2.1.3 Environmental Risk

Environment risk is defined as the probability that a substance or situation will produce harm over specific conditions. Risk is a combination of two factors: the probability that an adverse event will occur and the consequence of the adverse effect, (Presidential/Congressional Commission, 1997).

Allen and Shonnard (2002) analyzed the various aspects of how risk is assessed and described the environmental risk into three groups: voluntary risk, involuntary risk and natural disaster. The voluntary risk is normally associated with the known and quantifiable discharge of certain chemical into the air, water and terrain, while the involuntary is related to a release resulting from uncontrollable actions, such as system or equipment failures, and the natural disaster includes floods. earthquakes, and other disasters that are beyond human control.

The existing way of thinking about risk is that the plant from which emissions are analyzed is fixed, that is, the sizes of equipments are known and the level of operations (throughput) are also known. However, plants are subject to a) variable demand and consequently variable throughput, b) deteriorating equipment that affect performance and efficiency, c) fouling, d) other economic conditions that suggest a different operation, like for example, recycle a by-product more when its price goes down. All these suggest a variety of scenarios, for which second operational decisions (second stage decisions) are a function of the design variables (first stage decisions).

Using the solution from the stochastic planning problem one obtains new values of the expected environmental impact (θ) that represent the realization of the individual scenarios. These values are smaller than the indices obtained solving the scenario separately using the deterministic model. Therefore, the risk associated with each scenario is defined by:

$$Risk(x,\theta) = P(\theta(x) > \theta^*) \qquad (2.13)$$

Where θ = virtual environmental impact, and θ^* is the environmental impact aspiration level (minimum impact desired). As before, binary variables, similar to z_s are defined and a definition of environmental risk similar to financial risk is constructed.

Measuring the Process' Environmental Impact

Starting from the work by Mallick *et al.* (1996), the approach taken to measure the process' s environmental impact (θ) is the use of a non-monetary valuation technique that calculates the environmental impact of each chemical presented in the waste stream in term of environmental impact units (EIU) per kilogram of product produced.

$$\theta = (\sum_{i=1}^{n}\sum_{j=1}^{m} w_i m_{j,i} \Phi_j)/p \qquad (2.14)$$

where:

w_i = flow rate of waste stream i (kg/h)

$m_{j,i}$ = mass fraction of component j in waste stream i

Based on the work by Davis *et al.* (1994), the environmental impact index (Φ) is given by:

$$\Phi = (\text{Human health effect} + \text{environmental effect}) \times (\text{exposure potential}) \qquad (2.15)$$

$$\text{Human health effect} = HV_{oralD50} + HV_{inhalationLC50} + HV_{carcinogenity} + HV_{other} \qquad (2.16)$$

$$\text{Environmental effect} = HV_{oralD50} + HV_{fishLC50} + HV_{fishNOEL} \qquad (2.17)$$

$$\text{Exposure potential} = HV_{BOD} + HV_{hydrolisis} + HV_{BC} \tag{2.18}$$

where the hazard values HV_i for each end point i are calculated using toxicological information specific to each chemical as described by Davis et al. (1994).

For chronic terms, the carcinogenity and other specific effects, toxicological endpoints are calculated based on the classification presented in the hazard ranking system final rule (Federal Register, 1990) and in the Bouwes and Hassur (1997) methodology.

Subsequently, if these emissions, as well as other possible accidental release are not taken into account, the environmental impact of the process might not be correctly evaluated. In this context, a release factor (r) that accounts for the release potential of a particular stream – including waste and non-waste stream incorporated into later equation.

$$\theta = (\sum_{i=1}^{n}\sum_{j=1}^{m} r_i w_i m_{j,i} \Phi_j)/p \tag{2.19}$$

The release factor can take values from 0 to 1. For waste streams, r = 1, whereas for non-waste streams, 0<r<1,. Estimate r is equivalent to calculating the probability of obtaining a release from a specific stream. This can be done by considering past data and experiences related to the process under study or basing on the categories presented by Kolluru (1995), according to expected frequency of the release.

2.1.4 Uncertainty Sources

Table 2.1 Uncertainty sources (Dantus and High, 1999)

Type	Example
Process model uncertainty	Kinetic constants, physical properties, transfer coefficients
Process uncertainty	Flow rate and temperature variations, stream quality fluctuations
Economic model and environmental impact model uncertainty	Capital costs, manufacturing costs, direct costs, release factors, and less tangible costs
External uncertainty	Product demand, prices, feed stream availability, feed composition
Regulatory uncertainty	Modified emission standards, and new environment regulations
Time uncertainty	Investment delays (i.e. the project might have a better performance in the future)

2.2 Literature Survey

Grauer, Lewandowski & Wierzbiciki (1984) described methods for solving multiple-objective optimization problems by considering at multiple-objective decision analysis from the point of view of the type of optimization problems which must be solved in the design, control and production planning of chemical engineering systems as well as surveying existing methods. Moreover, they gave an overview of the existing software, provided an overview of computer codes (especially IIASA software) and discussed application in engineering field. In conclusion, they gave overview in the way of multiple-objective optimization.

During the past several decades, the use of integration techniques as a design tool to minimize the operating and capital costs of chemical plant has matured considerably and evolved into a common practice in the process industries. Also as a result of serious concerns about environmental problems in recent years, the multiple-objective programming (MOP) was applied to balance the economic and environmental effects. Chang & Hwang (1996) showed how they developed process integration methods for waste minimization in the utility systems of chemical process with maximization in economic. The study was to assess the feasibility and practical value of incorporating gas emission models into existing mathematical formulations and solving the resulting problem with multiple-objective optimization technique. One can conclude that the mixed-integer linear program (MILP) model is suitable for the design of a wide variety of utility systems; furthermore, the goal programming (GP) method is a natural and sensible design tool for establishing a compromise among conflicting objectives.

In 1999, Dantus & High studied about multiple-objective optimization approach under uncertainty in waste minimization. This work used two competing objectives: maximize profit and minimize the environmental impact. The former is measured by using the annual equivalent profit (AEP) tool and the latter using the environmental impact index. The AEP included the usual costs associated with the process, as well as the various waste related costs, for which a detailed discussion was given including the different ways available to estimate them. On the other hand, environmental impact index included toxicological characteristics of each chemical presented in the process stream and its release potential. Furthermore, they used stochastic programming with multiple-objective optimization technique to evaluate the uncertainty in optimizing the two competitive objectives. This accomplished using the process simulator ASPEN PLUS.

Then Lim, Floquet & Joulia (1999) discussed optimization of process by performing along an infeasible path with successive quadratic programming (SQP) algorithm. One of the objective functions, the global pollution index function, is based on environmental impact index calculated by using the hazard value (HV). The other is cost-benefit function. To analyze the bi-objective optimization, the noninferior solution curve (Pareto curve) was formed using summation of weighed objective function (SWOF), GP, and parameter space investigation (PSI) methods within a chemical process simulator. It can find the ideal compromise solution set based on the Pareto curve. The multi-objective problem was then interpreted by sensitivity and elasticity analyses of the Pareto curve that give the decision basis between the conflicting objectives.

For the similar method for optimization of multiobjective process planning under uncertainty, Rodera, Bagajewicz & Trafails (2002) presented that the single-objective MILP stochastic programming model could be treated as a multi-objective programming problem by using multi-parametric decomposition. The point estimate weighed-sums approach is one of the possible methods that can be used to obtain the set of efficient solution. This method makes use of the probabilities of each scenario to weight the respective objectives. However, because of the mixed-integer linear nature of the problem at hand, only supported efficient solutions are found by this method. Reformulation of the problem as an augmented weighed Tchebycheff program makes possible to computation of all efficient solutions. The objective is to scan the efficient frontier to provide the decision maker with the freedom to select the solution by aspiration levels. Different methods of specifying these aspiration levels are possible. This paper represented an iterative procedure based on the use of lower bound of the net present value that facilitates the assessment of economic risk of a project.

For the risk management, Barbaro & Begajewicz (2003) tried to develop new mathematical formulations for problems dealing with planning and design under uncertainty that allow management of financial risk according to the decision maker's preference. A major step toward this objective was the use of formal probabilistic definition of financial risk. In addition to this, the connection between down side risk and financial risk were discussed. Using two definitions, new two-stage stochastic programming models that are able to manage financial risk were developed. The advantages of the proposed approaches are that they maintain the original MILP structure of the problem. Comparisons with the robustness approach to risk management were made. It is shown that the probabilistic definition of the financial risk should be used to better capture the trade-off between expectation and variability of the objective function. Especially because the use of the upper partial mean may unnecessarily penalize favorable scenarios, resulting in non-optimal solutions that provide misleading information about the variability of the objective. The performance of these solutions obtained with the robustness approach from standpoint of financial risk was also discussed showing how solution that are considered "robust" may exhibit high levels of financial risk due to the non-optimality of the second-stage decisions.